Thermodynamics of the one-dimensional half-filled Hubbard model in the spin-disordered regime

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Abstract. We analyze the Thermodynamic Bethe Ansatz equations of the one-dimensional half-filled Hubbard model in the "spin-disordered regime", which is characterized by the temperature being much larger than the magnetic energy scale but small compared to the Mott–Hubbard gap. In this regime the thermodynamics of the Hubbard model can be thought of in terms of gapped charged excitations with an effective dispersion and spin degrees of freedom that only contribute entropically. In particular, the internal energy and the effective dispersion become essentially independent of temperature. An interpretation of this regime in terms of a putative interacting-electron system at zero temperature leads to a metal-insulator transition at a finite interaction strength above which the gap opens linearly. We relate these observations to studies of the Mott–Hubbard transition in the limit of infinite dimensions.

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1. Introduction

The Mott–Hubbard metal-insulator transition in the one-band Hubbard model at half band-filling continues to pose an intriguing problem [1, 2], even in the limit of infinite dimensions [3, 4]. Starting from the limit of large interactions, the Mott–Hubbard gap characterizing the insulating phase diminishes as U is lowered and eventually closes at a finite U_{c}. The determination of the precise value of the latter is an unsolved problem in infinite dimensions: The equations from Dynamical Mean-Field Theory need to be solved numerically and the best available treatments using the Dynamical Density-Matrix Renormalization Group method lead to conflicting results [5, 6].

Other attempts to determine U_{c} involve extrapolations of finite-order $1/U$-expansions of the Mott–Hubbard gap [7] and the ground-state energy [8], respectively. These expansions can be carried out because the spin background is completely disordered and one is left with finding the description of the effective motion of the charge degrees of freedom. However, the extrapolated values for U_{c} obtained by such methods vary significantly, depending on the details of the procedure.

In light of these issues it is desirable to have an example of a Hubbard-type model with a disordered spin background which can be solved exactly. One such example is the Falicov–Kimball model at half band-filling in the disordered phase [9]. However, its ground-state energy turns out to have a trivial $1/U$-expansion and hence is of limited utility. Curiously, the exactly solvable one-dimensional Hubbard model [10] at half band-filling features a spin-disordered regime at a small but finite temperature in the limit of strong Coulomb repulsion, see Refs. [11, 12, 13]. It is then an interesting question to analyze the physics of this regime in view of the above issues raised by the studies of the Mott–Hubbard insulator in infinite dimensions.

Our presentation is organized as follows. In section 2 we review the thermodynamics of the one-dimensional Hubbard model [14, 15, 16]. In section 3 we analyze the Thermodynamic Bethe Ansatz (TBA) equations in the spin-disordered regime and calculate the internal energy and the effective dispersion of the charge degrees of freedom. In section 4 we interpret these results in terms of a putative interacting-electron system at zero temperature. We conclude in section 5.

2. Thermodynamics of the one-dimensional Hubbard model

2.1. Hubbard model and TBA equations

The Hubbard model on L lattice sites is described by the Hamiltonian

$$\hat{H} = -t\sum_{j=1}^{L}\sum_{\sigma=\uparrow,\downarrow}(\hat{c}^{+}_{j,\sigma}\hat{c}_{j+1,\sigma} + \hat{c}^{+}_{j+1,\sigma}\hat{c}_{j,\sigma}) + U\sum_{j=1}^{L}(\hat{n}_{j,\uparrow} - 1/2)(\hat{n}_{j,\downarrow} - 1/2) \; . \quad (1)$$

In the following we define $u = U/(4t)$ and set $t = 1$ as our energy unit. Periodic boundary conditions apply, and the kinetic energy is diagonal in momentum space with the bare dispersion $\epsilon(k) = -2\cos k$.

The 'Thermodynamic Bethe Ansatz (TBA) equations' describe the ratios of the distributions of hole and particle excitations in thermal equilibrium at temperature T, chemical potential μ and magnetic field B ([14], eq. (5.60)-(5.65) of [10])

$$\begin{aligned}\ln\zeta(k) &= -\frac{2\cos k}{T} - \frac{4}{T}\int_{-\infty}^{\infty}\mathrm{d}\Lambda\ s(\sin k-\Lambda)\mathrm{Re}\left[\sqrt{1-(\Lambda-\mathrm{i}u)^2}\right] \\ &\quad + \int_{-\infty}^{\infty}\mathrm{d}\Lambda\ s(\sin k-\Lambda)\ln\left(\frac{1+\eta_1'(\Lambda)}{1+\eta_1(\Lambda)}\right) , \qquad (2)\\ \ln\eta_1(\Lambda) &= s*\ln(1+\eta_2)|_\Lambda - \int_{-\pi}^{\pi}\mathrm{d}k\cos(k)s(\Lambda-\sin k)\ln[1+1/\zeta(k)] , \\ \ln\eta_n(\Lambda) &= s*\ln(1+\eta_{n+1})(1+\eta_{n-1})|_\Lambda \qquad \text{for } n\geq 2 , \qquad (3)\end{aligned}$$

and likewise for $\eta_n'(\Lambda)$ with $1/\zeta(k)$ replaced by $\zeta(k)$. The convolution operation is defined by

$$\begin{aligned}s*f|_x &= \int_{-\infty}^{\infty}\mathrm{d}y\ s(x-y)f(y) , \\ s(x) &= \frac{1}{4u\cosh(\pi x/(2u))} = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{\exp(-\mathrm{i}\omega x)}{2\cosh(\omega u)} . \qquad (4)\end{aligned}$$

The "boundary conditions" are

$$\lim_{n\to\infty}\frac{\eta_n(\Lambda)}{n} = \frac{2B}{T} \quad , \quad \lim_{n\to\infty}\frac{\eta_n'(\Lambda)}{n} = -\frac{2\mu}{T} . \qquad (5)$$

2.2. Free-energy density and internal energy

In terms of the distribution functions $\zeta(k)$ and $\eta_1(\Lambda)$ the free-energy density can be cast into the form (see eq. (5.69) of [10])

$$f(T) = e_0-\mu-T\int_{-\pi}^{\pi}\mathrm{d}k\rho_0(k)\ln(1+\zeta(k))-T\int_{-\infty}^{\infty}\mathrm{d}\Lambda\sigma_0(\Lambda)\ln(1+\eta_1(\Lambda)) , \qquad (6)$$

where e_0 denotes the ground-state energy of the one-dimensional Hubbard model at half band-filling, see eq. (66). Here, the root densities $\sigma_0(\Lambda)$ and $\rho_0(k)$ are given by

$$\begin{aligned}\sigma_0(\Lambda) &= \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{J_0(\omega)\exp(-\mathrm{i}\omega\Lambda)}{2\cosh(\omega u)} , \\ \rho_0(k) &= \frac{1}{2\pi}+\cos k\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{J_0(\omega)\exp(-\mathrm{i}\omega\sin k)}{1+\exp(2u|\omega|)} , \qquad (7)\end{aligned}$$

and $J_n(x)$ are nth-order Bessel functions. With the help of (2) we can transform the free-energy density (6) into the form (see eq. (4.21) of [16])

$$f(T) \equiv C - T\alpha(T) - T\beta(T) , \qquad (8)$$

$$C = 4\int_{-\infty}^{\infty}\mathrm{d}\Lambda\sigma_0(\Lambda)\mathrm{Re}\left[\sqrt{1-(\Lambda-\mathrm{i}u)^2}\right] - u - \mu = -e_0-\mu , \qquad (9)$$

$$\alpha(T) = \int_{-\pi}^{\pi}\mathrm{d}k\rho_0(k)\ln(1+1/\zeta(k)) , \qquad (10)$$

$$\beta(T) = \int_{-\infty}^{\infty}\mathrm{d}\Lambda\sigma_0(\Lambda)\ln(1+\eta_1'(\Lambda)) . \qquad (11)$$

With the help of (8) the internal energy

$$e(T,u) = f(T) - T\frac{\partial f(T)}{\partial T} \tag{12}$$

can be expressed as

$$e(T,u) = C + T^2\left(\frac{\partial\alpha(T)}{\partial T} + \frac{\partial\beta(T)}{\partial T}\right) \ . \tag{13}$$

3. The spin-disordered limit

3.1. Definition of the limit

In the following we consider the TBA equations in the regime

$$J \ll T \ll \Delta \tag{14}$$

for $B = 0$ and $\mu = 0$, i.e., the half-filled Hubbard chain in zero magnetic field. Here, $J(U/t \to \infty) = 4t^2/U$ is the coupling strength for the spin degrees of freedom, and Δ is the gap for charge excitations, $\Delta(U/t \to \infty) = U - 4t$. The inequalities (14) imply that

$$\frac{1}{UT} \ll 1 \quad , \quad \exp\left(-\frac{U}{T}\right) \ll 1 \ . \tag{15}$$

In this limit, the spin degrees of freedom are 'hot', i.e., the charge degrees of freedom move in a random spin background.

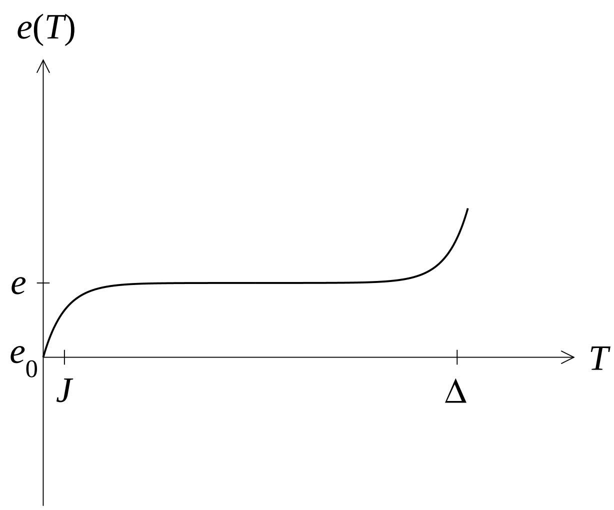

Figure 1. Internal energy as a function of temperature for the Hubbard model at half band-filling and large interactions.

The qualitative dependence of the internal energy as a function of temperature is shown in Fig. 1. In the temperature range given by (14) the internal energy is essentially independent of temperature because the spin degrees of freedom contribute maximally to the internal energy whereas there are exponentially few charge excitations.

3.1.1. Charge sector We define the *dressed energy* for charge excitations by

$$\kappa(k,u,T) = T\ln(\zeta(k)) \ . \tag{16}$$

We will see that, in the spin-disordered regime, the dressed energy has an expansion of the form

$$\kappa(k,u,T) = \sum_{m=0}^{\infty}\left(\frac{1}{uT}\right)^m \kappa^{(m)}(k,u) + \mathcal{O}(e^{-u/T}) \ . \tag{17}$$

The leading term in this expansion is temperature independent, negative and of order $\mathcal{O}(u)$. Hence

$$\zeta(k) = \mathcal{O}(e^{-u/T}) \ll 1 \ , \tag{18}$$

$$\ln(1+1/\zeta(k)) = -\ln(\zeta(k)) + \mathcal{O}(e^{-u/T}) \ . \tag{19}$$

Equation (19) leads to a significant simplification of the TBA equations.

3.1.2. k-Λ Strings Neglecting terms of order $\mathcal{O}(e^{-u/T})$, the TBA equations for k-Λ strings take the form

$$\ln\eta'_n(\Lambda) = \ s * \ln(1+\eta'_{n+1})(1+\eta'_{n-1})\Big|_{\Lambda} \ , \tag{20}$$

where we define $\eta'_0(\Lambda) = 0$. The solution to (20) under the boundary conditions (5) with $\mu = 0$ is [14]

$$\eta'_n(\Lambda) = (n+1)^2 - 1 \ . \tag{21}$$

The corrections to η' are of order $\exp\Big(\exp(-u/T)\Big)$.

3.1.3. Λ Strings Neglecting terms of order $\mathcal{O}(e^{-u/T})$, the TBA equations for Λ strings take the form

$$\ln\eta_n(\Lambda) = \ s * \ln(1+\eta_{n+1})(1+\eta_{n-1})\big|_{\Lambda} \ , \tag{22}$$

where we define

$$\eta_0(\Lambda) = \exp\left(-\frac{4}{T}\mathrm{Re}\sqrt{1-\Lambda^2}\right) - 1 \ . \tag{23}$$

The solution to (22) under the boundary conditions (5) with $B = 0$ can be obtained by iterative linearization, as shown in Ref. [16]. The starting point is the solution $\eta_n^{(0)}$ to the equations (22) with $\eta_0 = 0$, i.e.,

$$\eta_n^{(0)}(\Lambda) = (n+1)^2 - 1 \ . \tag{24}$$

One then linearizes (22) around the solution (24) by writing $\eta_n = \eta_n^{(0)} + \eta_n^{(1)}$ (for $n \geq 1$) and keeping only the terms linear in $\eta_n^{(1)}$. This gives the following set of linear integral equations

$$\frac{\eta_n^{(1)}}{\eta_n^{(0)}} = s * \frac{\eta_{n-1}^{(1)}}{1+\eta_{n-1}^{(0)}} + s * \frac{\eta_{n+1}^{(1)}}{1+\eta_{n+1}^{(0)}} \ . \tag{25}$$

The boundary conditions are given by (5) and

$$\eta_0^{(1)}(\Lambda) = -\frac{4}{T}\mathrm{Re}\sqrt{1-\Lambda^2}\ . \tag{26}$$

The set of linear integral equations (25) can be solved by Fourier transform [16]. We find

$$\begin{aligned}\eta_n^{(1)}(\Lambda) &= \frac{2(n+1)n}{T}\mathrm{Re}\left[\sqrt{1-(\Lambda-\mathrm{i}u(n+2))^2}\right]\\ &\quad -\frac{2(n+1)(n+2)}{T}\mathrm{Re}\left[\sqrt{1-(\Lambda-\mathrm{i}nu)^2}\right]\\ &= \mathcal{O}\left(\frac{1}{uT}\right)\ .\end{aligned} \tag{27}$$

We see that we have

$$|\eta_1^{(1)}(\Lambda)| \ll \eta_1^{(0)}(\Lambda) = 3\ , \tag{28}$$

as required.

3.2. Dressed energy of the charge degrees of freedom

Combining the results for $\eta_1(\Lambda)$ and $\eta_1'(\Lambda)$ we obtain

$$\ln\left[\frac{1+\eta_1'(\Lambda)}{1+\eta_1(\Lambda)}\right] \approx -\frac{1}{4}\eta_1^{(1)}(\Lambda)\ . \tag{29}$$

Substituting this back into (2) we obtain the first term of the expansion (17)

$$\kappa^{(0)}(k,u) = -2\cos k - 2u - \frac{1}{2}\int_{-\infty}^{\infty}\frac{d\omega}{\omega}J_1(\omega)e^{\mathrm{i}\omega\sin k}e^{-2u|\omega|}\ . \tag{30}$$

Crucially, the contributions of η_1 and η_1' to $\zeta(k)$ do not feed back into the integral equations for η_n and η_n'. The reasons for this are that

(i) the corrections do not change the fact that ζ is $\mathcal{O}(\exp(-u/T))$ and terms involving $\ln(1+\zeta(k))$ can therefore be dropped from the TBA equations;

(ii) the corrections to $\ln(\zeta)$ depend only on $\sin(k)$ and therefore do not contribute to

$$\int_{-\pi}^{\pi}\mathrm{d}k\cos(k)\ s(\Lambda-\sin k)\ln[\zeta(k)]\ . \tag{31}$$

The result (30) should be compared to the corresponding expression at zero temperature, see eq. (7.10) of [10],

$$\kappa_0(k,u) = -2\cos k - 2u - 2\int_{-\infty}^{\infty}\frac{d\omega}{\omega}J_1(\omega)e^{\mathrm{i}\omega\sin k}\frac{1}{1+\exp(2|\omega|u)}\ . \tag{32}$$

Performing the integral in (30) we finally find ($u=U/4$)

$$\kappa^{(0)}(k,U) = \epsilon(k) - \frac{1}{2\sqrt{2}}\sqrt{[\epsilon(k)]^2+U^2+\sqrt{[\epsilon(k)^2-U^2]^2+(4U)^2}}\ , \tag{33}$$

where $\epsilon(k) = -2\cos k$ is the bare dispersion.

The interesting point is that $\kappa^{(0)}(k) \neq \kappa_0(k)$ despite the fact that $T \ll |\kappa_0(k)|$. The reason for this is that spin and charge degrees of freedom are still coupled in the

Hubbard model. This is obvious from the TBA equations and also from the known scattering matrix of elementary excitations [17], see Chap. 7.4 in [10]. We note that the modification of the dressed energy of the charge degrees of freedom by the spin sector is a general characteristic of the spin-disordered regime. In the asymptotic low-energy regime, spin and charge degrees of freedom decouple quite generically for one-dimensional interacting-electron systems. However, on the scale of the temperature in the spin-disordered regime such a decoupling no longer holds. This in turn is expected to lead to modifications in non-universal physical properties such as the charge velocity. Our result is in agreement with this expectation which we note equally applies to a less than half-filled band.

3.3. Dressed momentum of the charge degrees of freedom

The total momentum in thermal equilibrium is equal to zero by virtue of translational invariance. In order to determine the dressed momentum of our charge excitation, we start from the expression for the contribution of a charge excitation with real k's to the total momentum [18] (see (5.97) and (5.38) of [10])

$$p(k) = k + \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\Lambda \theta \left(\frac{\sin k - \Lambda}{nu} \right) \left[\sigma_n'^p(\Lambda) + \sigma_n^p(\Lambda) \right] \ , \tag{34}$$

where

$$\theta(x) = 2 \arctan(x) \tag{35}$$

and the root densities for particles and holes obey (see (5.41) of [10])

$$\rho^p(k) + \rho^h(k) = \frac{1}{2\pi} + \cos k \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} \mathrm{d}\Lambda a_n(\sin k - \Lambda) \left[\sigma_n'^p(\Lambda) + \sigma_n^p(\Lambda) \right] \ , \tag{36}$$

$$\begin{aligned} \sigma_n^p(\Lambda) &= -\sigma_n^h(\Lambda) + s * \left(\sigma_{n+1}^h + \sigma_{n-1}^h \right)\Big|_\Lambda \\ &\quad + \delta_{n,1} \int_{-\pi}^{\pi} \mathrm{d}k s(\Lambda - \sin k) \rho^p(k) \ , \end{aligned} \tag{37}$$

$$\begin{aligned} \sigma_n'^p(\Lambda) &= -\sigma_n'^h(\Lambda) + s * \left(\sigma_{n+1}'^h + \sigma_{n-1}'^h \right)\Big|_\Lambda \\ &\quad - \delta_{n,1} \int_{-\pi}^{\pi} \mathrm{d}k s(\Lambda - \sin k) \left(\rho^p(k) - \frac{1}{2\pi} \right) \end{aligned} \tag{38}$$

with

$$\eta_n(\Lambda) = \frac{\sigma_n^h(\Lambda)}{\sigma_n^p(\Lambda)} \quad , \quad \eta_n'(\Lambda) = \frac{\sigma_n'^h(\Lambda)}{\sigma_n'^p(\Lambda)} \quad , \quad \zeta(k) = \frac{\rho^h(k)}{\rho^p(k)} \ . \tag{39}$$

As $\zeta(k) = \mathcal{O}(\exp(-u/T))$ we can drop $\rho^h(k)$ from equation (36) and substitute the resulting equation into (37) and (38). We obtain the following result for the driving term

$$\int_{-\pi}^{\pi} \mathrm{d}k s(\Lambda - \sin k) \rho^p(k) = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} s(\Lambda - \sin k) = \sigma_0(\Lambda) \ . \tag{40}$$

The temperature-independent contribution to the particle and hole root densities is obtained by using (21) and (24) and then solving the resulting sets of coupled linear integral equations. We find

$$\sigma_n^{\prime p,h}(\Lambda) = \mathcal{O}\left(\exp(-u/T)\right) \tag{41}$$

and

$$\begin{aligned}\sigma_n^{p}(\Lambda) =& \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{J_0(\omega)\exp\left(-\mathrm{i}\omega\Lambda\right)}{2(n+1)} \left[\frac{\exp(-nu|\omega|)}{n} - \frac{\exp(-(n+2)u|\omega|)}{n+2}\right] \\ &+ \mathcal{O}\left(\exp(-u/T)\right) \qquad (42)\\ =& -\frac{1}{2\pi(n+1)(n+2)}\mathrm{Re}\left(\frac{1}{\sqrt{1-(\Lambda-\mathrm{i}(n+2)u)^2}}\right) \\ &+ \frac{1}{2\pi n(n+1)}\mathrm{Re}\left(\frac{1}{\sqrt{1-(\Lambda-\mathrm{i}nu)^2}}\right) + \mathcal{O}\left(\exp(-u/T)\right) . \qquad (43)\end{aligned}$$

Substituting (43) back into (34) we obtain the temperature-independent contribution to the dressed momentum

$$p(k) = k + \frac{1}{2}\arcsin\left[\frac{2\sin k}{\sqrt{4u^2+(\sin k+1)^2}+\sqrt{4u^2+(\sin k-1)^2}}\right] . \tag{44}$$

We note that the physical momenta of holons (h) and anti-holons ($\overline{h}$) are obtained from $p(k)$ by $p_h(k) = \pi/2 - p(k) = p_{\overline{h}}(k) + \pi$.

3.4. Effective dispersion for strong coupling

The effective dispersion is given implicitly by equations (33) and (44). In order to have a consistent expansion for the Hubbard model in the spin-disordered regime, we need to truncate these two equations at order $1/u$ because the next subleading temperature-dependent contributions are of the order $1/(uT)$. Hence, the effective dispersion in the spin-disordered Hubbard model is given by

$$\kappa^{(0)}(p,u) = -2u - 2\cos p - \frac{1}{4u}(3-2\cos^2 p) + \mathcal{O}\left(u^{-2}\right) . \tag{45}$$

For the Hubbard model at zero temperature we find instead

$$\kappa_0(p,u) = -2u - 2\cos p - \frac{\ln 2}{u}(3-2\cos^2 p) + \mathcal{O}\left(u^{-2}\right) . \tag{46}$$

Both formulae can be cast into the form

$$\kappa(p,u,T) = -2u - 2\cos p - \frac{1}{4u}\left(1-4\gamma_{\mathrm{s}}(T)\right)(3-2\cos^2 p) + \mathcal{O}\left(u^{-2}\right) , \tag{47}$$

where

$$\gamma_{\mathrm{s}}(T) = \langle \hat{\mathbf{S}}_i \hat{\mathbf{S}}_{i+1}\rangle_{\mathrm{s}} \tag{48}$$

denotes the nearest-neighbor spin correlation function in the Heisenberg model at temperature T. Thermal averages of operators $\hat{A}$ over spin configurations are defined by

$$\langle \hat{A} \rangle_{\rm s} = \frac{{\rm Tr}\left[\exp\left(-\beta \hat{H}_{\rm Heis}\right)\hat{A}\right]}{{\rm Tr}\left[\exp\left(-\beta \hat{H}_{\rm Heis}\right)\right]} \tag{49}$$

with the Heisenberg Hamiltonian (see Appendix 2.A of [10])

$$\hat{H}_{\rm Heis} = \sum_i \frac{4t^2}{U}\left(\hat{\mathbf{S}}_i\hat{\mathbf{S}}_{i+1} - \frac{1}{4}\right) . \tag{50}$$

In fact, we have $\gamma_{\rm s}(T = 0) = 1/4 - \ln(2)$ from the Bethe-Ansatz solution of the Heisenberg model [19] and $\gamma_{\rm s}(T = \infty) = 0$ for uncorrelated spins. Results for all temperatures can be found in Refs. [20, 21].

The result (47) can be obtained within the $1/U$-expansion [7]. This approach can be used here because the one-dimensional lattice is a Bethe lattice with coordination number $Z = 2$. To leading order in $1/u$ we must treat the Hamiltonian

$$\hat{h}_1 = -\frac{1}{U}\hat{P}_0\hat{T}\hat{P}_1\hat{T}\hat{P}_0 , \tag{51}$$

where $\hat{P}_0$ projects onto the subspace of zero double occupancies. At half band-filling, $\hat{h}_1$ reduces to the Heisenberg model (50). The internal energy density of the Heisenberg model is given by

$$e_{\rm s}(T) = \frac{1}{u}\left(\gamma_{\rm s}(T) - \frac{1}{4}\right) , \tag{52}$$

and can be calculated analytically in terms of the Thermodynamic Bethe Ansatz [15, 22] or, equivalently, via the solution of a set of coupled integral equations [23].

For the derivation of the effective dispersion we have to solve (see (43) of [7])

$$\begin{aligned}\frac{U}{L}\sum_{j,\sigma}\left\langle \hat{c}_{j,\sigma}^{+}\left(\hat{h}_1 - Le_{\rm s}(T)\right)\hat{c}_{j,\sigma}\right\rangle_{\rm s} &= \frac{1}{L}\sum_{j,\sigma}\left\langle \hat{c}_{j,\sigma}^{+}\left[g_{1,2}(\hat{h}_0)^2 + g_{1,0}\right]\hat{c}_{j,\sigma}\right\rangle_{\rm s} \\ &= 2g_{1,2} + g_{1,0} ,\end{aligned} \tag{53}$$

where $\hat{h}_0$ describes the the hopping of holes in the spin background, $\hat{h}_0 = \hat{P}_0\hat{T}\hat{P}_0$. The expectation value on the left-hand-side of (53) is readily calculated so that we find

$$-8\left(\gamma_{\rm s}(T) - \frac{1}{4}\right) = 2g_{1,2} + g_{1,0} \tag{54}$$

as our first equation. The second equation we obtain from the solution of eq. (44) of [7],

$$\begin{aligned}&\frac{U}{L}\sum_{j,\sigma}\left\langle \hat{c}_{j,\sigma}^{+}\left(\hat{h}_1 - Le_{\rm s}(T)\right)(\hat{h}_0)^2\hat{c}_{j,\sigma}\right\rangle_{\rm s} \\ &\qquad = \frac{1}{L}\sum_{j,\sigma}\left\langle \hat{c}_{j,\sigma}^{+}\left[g_{1,2}(\hat{h}_0)^2 + g_{1,0}\right](\hat{h}_0)^2\hat{c}_{j,\sigma}\right\rangle_{\rm s} \\ &\qquad = 6g_{1,2} + 2g_{1,0} .\end{aligned} \tag{55}$$

The expectation value on the left-hand-side of (55) is readily calculated and we find

$$4\left(\gamma_{\rm s}(T) - \frac{1}{4}\right) = 2g_{1,2} \tag{56}$$

as our second equation. From this $g_{1,2} = -(1-4\gamma_{\rm s}(T))/2$ and $g_{1,0} = 3(1-4\gamma_{\rm s}(T))$ result, and the effective Hamiltonian for the motion of a single hole in a spin background becomes

$$\hat{h}^{\rm eff} = \hat{h}_0 + (1-4\gamma_{\rm s}(T))\frac{\left(-(\hat{h}_0)^2/2+3\right)}{U} + \mathcal{O}\left(U^{-2}\right) . \tag{57}$$

Replacing $\hat{h}_0 \to -\epsilon(p) = 2\cos p$ and $\omega + 2u = -\hat{h}^{\rm eff}$ as in [7] we find for $\kappa(p,u,T) \equiv \omega$

$$\kappa(p,u,T) = -2u - 2\cos p - \frac{1}{4u}(1-4\gamma_{\rm s}(T))(3-2\cos^2 p) + \mathcal{O}\left(u^{-2}\right) , \tag{58}$$

as used in (47).

From the $1/U$-expansion we can determine the density of states of the lower Hubbard band. As in [7] the shape-correction factor to first order is found to be $s(\epsilon) = 1-(1-4\gamma_{\rm s}(T))\epsilon/U$ so that we find $[\alpha(T) = 1-4\gamma_{\rm s}(T)]$

$$\begin{aligned} D^{(1)}_{\rm LHB}(\omega) = & \int_{-2}^{2} {\rm d}\epsilon \rho_0(\epsilon)\left(1-\alpha(T)\frac{\epsilon}{U}\right)\delta\left(\omega + U/2 + \epsilon + \alpha(T)\frac{6-\epsilon^2}{2U}\right) \\ & = \rho_0\left[\left(U - \sqrt{(1+\alpha(T))U^2 + 2\alpha(T)U\omega + 6\alpha(T)^2}\right)/\alpha(T)\right] , \end{aligned} \tag{59}$$

where $\rho_0(\epsilon) = 1/(\pi\sqrt{4-\epsilon^2})$ for $|\epsilon| < 2$ is the density of states for non-interacting electrons and $\omega_- < \omega < \omega_+$ with $\omega_\pm = -U/2 \pm 2 - \alpha(T)/U$. In particular, for the single-particle gap we find

$$\Delta^{(1)}(u,T) = -2\omega_+ = 4u - 4 + \frac{1-4\gamma_{\rm s}(T)}{2u} , \tag{60}$$

up to and including the first order in the strong-coupling expansion.

Finally, we note that the momentum distribution can also be determined along these lines. We find

$$\langle \hat{n}_p \rangle_{\rm s} = \sum_\sigma \langle \hat{n}_{p\sigma}\rangle_{\rm s} = 1 - \frac{\cos p}{2u}(1-4\gamma_{\rm s}(T)) + \mathcal{O}\left(u^{-2}\right) , \tag{61}$$

in agreement with eq. (3.2) of Ref. [24].

3.5. Internal energy

We must evaluate (13) in the spin-disorder limit. We have

$$e_\alpha \equiv T^2\frac{\partial\alpha}{\partial T} \approx \int_{-\pi}^{\pi} {\rm d}k\rho_0(k)\kappa^{(0)}(k,u) , \tag{62}$$

$$e_\beta \equiv T^2\frac{\partial\beta}{\partial T} = 0 . \tag{63}$$

The latter follows from the fact that η_1' is independent of temperature. This leads to the following expression for the internal energy

$$\begin{aligned} e(T,u) = & -u - \int_0^\infty \frac{{\rm d}\omega}{\omega} J_0(\omega)J_1(\omega)\exp(-2u\omega) + \mathcal{O}(1/Tu) \\ = & -\frac{2u}{\pi}{\rm E}\left(-\frac{1}{u^2}\right) + \mathcal{O}(1/Tu) \equiv e(u) + \mathcal{O}(1/Tu) . \end{aligned} \tag{64}$$

From the internal energy we can derive the average double occupancy, $d(u) = (1/4)(\partial[e(T,u)+u])/(\partial u)$, as

$$d(u) = \frac{1}{4} - \frac{1}{2\pi}\mathrm{K}\left(-\frac{1}{u^2}\right) + \mathcal{O}(1/Tu)\,. \tag{65}$$

Here $\mathrm{K}(m)$ and $\mathrm{E}(m)$ are the complete elliptic integrals of the first and second kind, respectively. The internal energy is to be compared to the ground-state energy of the Hubbard model at half band-filling

$$e_0(u) = -u - 4\int_0^\infty \frac{\mathrm{d}\omega}{\omega} J_0(\omega)J_1(\omega)\frac{1}{1+\exp(2u\omega)}\,. \tag{66}$$

The average double occupancy for the Hubbard model at zero temperature follows from the derivative of (66) with respect to the interaction strength.

4. Zero-temperature interpretation

4.1. Mott–Hubbard transition

Now we *interpret* our results in terms of a putative one-dimensional interacting-electron system at zero temperature. In practice, we use the results for the temperature-independent contributions to the internal energy and the effective dispersion derived for the spin-disorder regime in the Hubbard model, $J \ll T \ll \Delta$, for *any* value of U. Our motivation are studies of the Hubbard model in infinite dimensions where the Mott–Hubbard insulator is in the spin-disordered phase above the Mott–Hubbard transition. In order to model such a situation in a one-dimensional system one would need to take the limit $T \to 0$ *after* letting $J \to 0$. Of course, this is not possible for the Hubbard model.

The one-dimensional Hubbard model at half band-filling describes a Mott–Hubbard insulator for all $U > 0$, i.e., the gap $\Delta_0(U)/2$ for single-particle charge excitations is finite, $\Delta_0(U) = -2\kappa_0(\pm\pi, U)$. From (32) we have

$$\Delta_0(U) = 2\left[-2 + \frac{U}{2} + 4\int_0^\infty \frac{\mathrm{d}\omega}{\omega} J_1(\omega)\frac{1}{1+\exp(U\omega/2)}\right]\,. \tag{67}$$

For $U \to 0$, the gap is exponentially small whereas it increases linearly with U for large interactions. The transition at $U_{\mathrm{c}} = 0^+$ is readily understood as the consequence of the perfect-nesting property in one dimension so that the (marginally) relevant Umklapp scattering processes drive the system into the insulating phase for all $U > 0$.

In our putative interacting-electron system these scattering processes are rendered ineffective by the random spin background which, at zero energy cost, provides a mechanism to dissipate momentum in scattering processes involving charge degrees of freedom. Therefore, we expect that the charge gap will open at a critical interaction strength. Indeed, from (30) and (33) we find

$$\Delta(U) = 2\left[-2 + \frac{U}{2} + \int_0^\infty \frac{\mathrm{d}\omega}{\omega} J_1(\omega)\exp(-U\omega/2)\right] = -4 + \sqrt{U^2+4}\,. \tag{68}$$

The gap opens linearly with slope $\sqrt{3}/2$ at

$$U_{\rm c} = 2\sqrt{3} = \frac{\sqrt{3}}{2}W \approx 0.866W \;, \tag{69}$$

where $W = 4$ is the bandwidth of the Hubbard model. The gap is shown in Fig. 2.

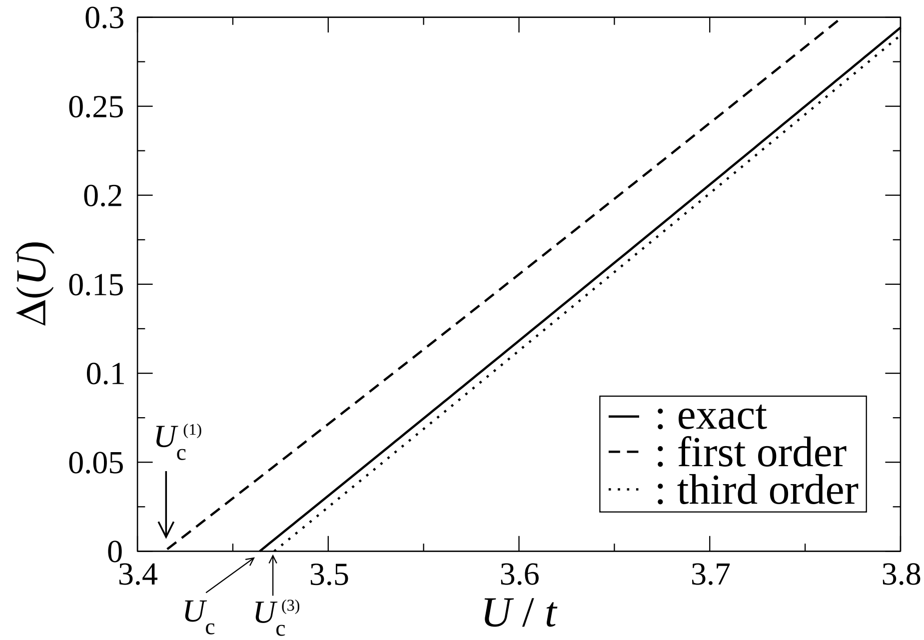

Figure 2. Gap for single-particle excitations as a function of the interaction strength U for the interacting-electron system with a disordered spin background at half band-filling.

4.2. Average double occupancy

We expect that physical quantities such as the average double occupancy display unphysical behaviour in the region $U < U_{\rm c}$. In fact, $d(u)$ contains a term proportional to $u \ln(u)$ so that its derivative diverges logarithmically for $u \to 0$. This diverging slope is seen in Fig. 3 where we compare the average double occupancy of the interacting-electron system with a spin-disordered background with the double occupancy of the Hubbard model.

4.3. Strong-coupling expansions

The internal energy of the Hubbard model at zero temperature and in the spin-disordered case can be expanded in powers of $1/U$. In both cases, the radius of convergence is given by $U_{\rm R}^{\rm e} = 4$, see (6.83) of [10] for $e_0(u)$ and (17.3.12) of [25] for $e(u)$. Explicitly,

$$\begin{aligned}[e(U)+U/4]/U &= \sum_{m=1}^{\infty} a_{2m} U^{-2m} \\ &= -\frac{1}{U^2} + \frac{3}{U^4} - \frac{20}{U^6} + \frac{175}{U^8} - \frac{1764}{U^{10}} + \frac{19404}{U^{12}} \pm \cdots \;. \end{aligned} \tag{70}$$

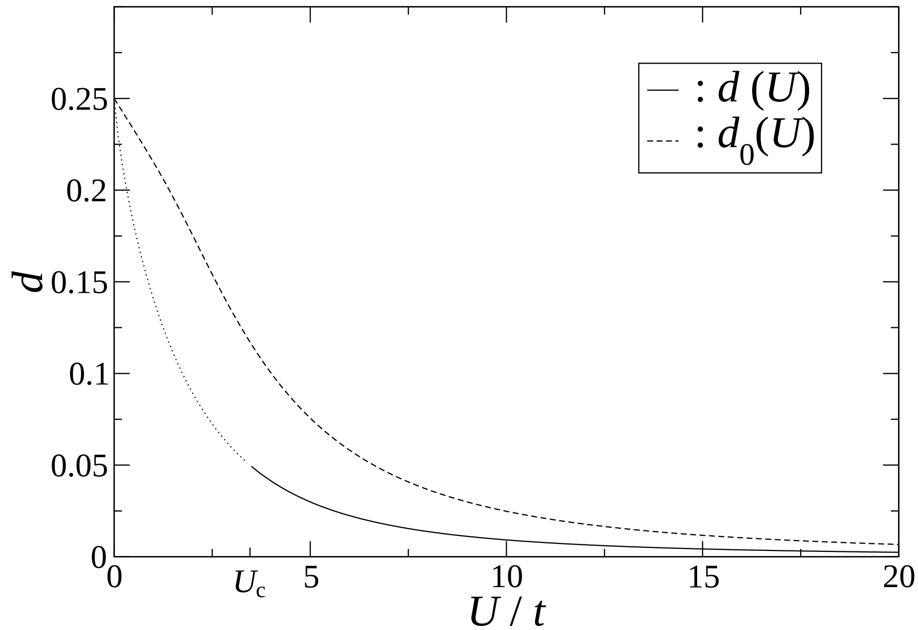

Figure 3. Average double occupancy $d_0(U)$ of the Hubbard model at half band-filling as compared to $d(U)$ (65) for the interacting-electron system with a spin-disordered background.

In (52) we determined the coefficient $a_2 = -1$ within the $1/U$-expansion. From the coefficients a_{2m}, one may actually deduce the radius of convergence of the series, as done in [8], by extrapolating the ratio of the coefficients $r(m) = |a_{2m}/a_{2m-2}|$ $(m \geq 2)$ for $m \to \infty$. In our case $r(m) = 4(2m-1)(2m-3)/m^2$ is a second-order polynomial in $1/m$ and we correctly find

$$U_{\mathrm{R}}^{\mathrm{e}} = \lim_{m\to\infty} \left(\sqrt{r(m)}\right) = 4 \; . \tag{71}$$

Note, however, that the radius of convergence of the energy is not related to the critical interaction strength of the metal-insulator transition, $U_{\mathrm{c}} = 2\sqrt{3}$. Therefore, it may also be doubted that this approach [8] is justified for the case of the infinite-dimensional Hubbard model.

In contrast to the internal energy, the series expansion of the gap in the spin-disordered Hubbard model converges for $U > U_{\mathrm{R}}^{\mathrm{gap}} = 2$. The first terms of the expansion read

$$\Delta(U) = \sum_{m=-1}^{\infty} b_m U^{-m} = U - 4 + \frac{2}{U} - \frac{2}{U^3} \pm \cdots \; . \tag{72}$$

In (60) we determined the coefficients $b_{-1} = 1$, $b_0 = 4$, and $b_1 = 2$ within the $1/U$-expansion.

Now that $U_{\mathrm{c}} = 2\sqrt{3}$ is larger than the convergence radius of the series, $U_{\mathrm{R}}^{\mathrm{gap}} = 2$, the gap opens linearly and the first few orders of the $1/U$-expansion provide a good description of the gap, as shown in Fig. 2. This is particularly true for the critical values for the closing of the gap as inferred from the truncated $1/U$-expansion. Let us

denote by $\Delta^{(m)}(U)$ the mth-order truncation of the series, e.g.,

$$\begin{aligned}
\Delta^{(0)}(U) &= U - 4 \, , \\
\Delta^{(1)}(U) &= U - 4 - \frac{2}{U} \, , \\
\Delta^{(3)}(U) &= U - 4 - \frac{2}{U} - \frac{2}{U^3} \, ,
\end{aligned} \tag{73}$$

etc., and let $U_{\mathrm{c}}^{(m)}$ be the critical interaction strength at which the mth gap opens, $\Delta^{(m)}(U_{\mathrm{c}}^{(m)}) = 0$. We then find

$$\begin{aligned}
U_{\mathrm{c}}^{(0)} &= 4 \, , \\
U_{\mathrm{c}}^{(1)} &= 3.4142[1.4\%] \, , \\
U_{\mathrm{c}}^{(3)} &= 3.4717[0.2\%] \, , \\
&\vdots \\
U_{\mathrm{c}} \;\; &= 2\sqrt{3} = 3.4651 \, .
\end{aligned} \tag{74}$$

The numbers in square brackets give the percentage difference to U_{c}. It is seen that the series converges very fast to the exact value. This observation supports the application of this approach to the Hubbard model in infinite dimensions [5, 7].

5. Conclusions

We have analyzed the Thermodynamic Bethe Ansatz equations for the half-filled one-dimensional Hubbard model in the spin-disordered regime, $t^2/U \ll T \ll U$. We have derived explicit expressions for the leading terms in the internal energy and the dressed energy and momentum of the charge degrees of freedom. The resulting effective dispersion of holons and anti-holons differs from the corresponding result in the half-filled Hubbard model at zero temperature to order $J = 4t^2/U$. This effect is due to the coupling of charge and spin degrees of freedom and occurs at the expected energy scale.

We then interpreted the entire temperature-independent part of the effective dispersion and the internal energy in terms of a putative interacting-electron system at zero temperature. From these results we derived some implications for the analysis of large-coupling expansions for the Mott–Hubbard insulator in infinite dimensions. Moreover, our analytical result can be used to assess the quality of other approximate schemes which describe the effective charge dispersion in a random spin background, see, e.g., Ref. [26].

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References

[1] N F Mott, *Metal–Insulator Transitions*, 2nd edition (Taylor and Francis, London, 1990).
[2] F Gebhard, *The Mott Metal-Insulator Transition* (Springer, Berlin, 1997).
[3] W Metzner and D Vollhardt, Phys. Rev. Lett. **62**, 324 (1989).
[4] A Georges, G Kotliar, W Krauth, and M J Rozenberg, Rev. Mod. Phys. **68**, 13 (1996).
[5] S Nishimoto, F Gebhard, and E Jeckelmann, J. Phys. Cond. Matt. **16**, 7063 (2004).
[6] M Karski, C Raas, and G S Uhrig, Phys. Rev. B **72**, 113110 (2005).
[7] M P Eastwood, F Gebhard, E Kalinowski, S Nishimoto, and R M Noack, Eur. Phys. J. B **35**, 155 (2003).
[8] N Blümer and E Kalinowski, Phys. Rev. B **71**, 195102 (2005).
[9] J K Freericks and V Zlatic, Rev. Mod. Phys. **75**, 1333 (2003).
[10] F H L Essler, H Frahm, F Göhmann, A Klümper, and V E Korepin, *The one-dimensional Hubbard model* (Cambridge University Press, Cambridge, 2005).
[11] F Gebhard, K Bott, M Scheidler, P Thomas, and S W Koch, Phil. Mag. B **75**, 13 (1997).
[12] V V Cheianov and M B Zvonarev, Phys. Rev. Lett. **92**, 176401 (2004).
[13] G A Fiete and L Balents, Phys. Rev. Lett. **93**, 226401 (2004).
[14] M Takahashi, Prog. Theor. Phys. **47**, 69 (1972); Prog. Theor. Phys. **52**, 103 (1974).
[15] M Takahashi, *Thermodynamics of One-Dimensional Solvable Models* (Cambridge University Press, Cambridge, 1999).
[16] Z N C Ha, Phys. Rev. B **46**, 12205 (1992).
[17] F H L Essler and V E Korepin, Phys. Rev. Lett. **72**, 908 (1994); Nucl. Phys. B **426**, 505 (1994).
[18] F Woynarovich, J. Phys. C **15**, 97 (1982); *ibid.*, 6397 (1982).
[19] H Bethe, Z. Phys. **71**, 205 (1931); see also eq. (6.83) of [10].
[20] Z Tsuboi and M Shiroishi, J. Phys. A **38**, L363 (2005).
[21] M Bortz and F Göhmann, Eur. Phys. J. B **46**, 399 (2005).
[22] M Takahashi, Prog. Theor. Phys. **46**, 401 (1971).
[23] A Klümper, Z. Phys. **91**, 507 (1993).
[24] M Takahashi, J. Phys. C **10**, 1289 (1977).
[25] M Abramovitz and I A Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1972).
[26] A Reischl, E Müller-Hartmann, and G S Uhrig, Phys. Rev. B **70**, 245124 (2004).